Case Study

Mass Spectrometry

The scientific field of Mass Spectrometry (MS) has been under constant research and development for over a hundred years, ever since scientists discovered that charged particles could be separated via electromagnetic fields based on their charge-to-mass ratio (Q/m). While spectrometry systems now come in numerous configurations their performance largely depends on a few fundamental elements. In the modern Mass Spectrometer this is normally the ion source (for exciting ions from the material under analysis), the mass analyzer, the particle detector and its associated electronics.

REMPI Application

In Mass Spectrometry the ion source plays a key role in determining the type of sample that can be analyzed by a particular spectrometer. One technique that offers great potential for the pharmaceutical industry is resonance-enhanced multi-photon ionization (REMPI). REMPI is a laser-based gas phase spectroscopy combined with ab initio calculations generating precise structural information on molecules such as neurotransmitters. The result is a rigorous platform for understanding the molecule behavior and ultimately, rationalizing drug design. The resonant two photon ionization technique allows electronic (and IR) spectra to be measured for molecules cooled to a few degrees Kelvin. This results in beautiful, simplified spectra that can be interpreted in terms of the possible conformers of the molecule.

The technique relies on a time-of-flight mass spectrometer, where particular ions are selected based on their arrival time. Figure 1 shows a REMPI MS system developed at Latrobe University, Melbourne, Australia.

This instrument uses a Spectrum 250 MS/s, 14 bit PCIe digitizer (model M3i.4121-exp) for data collection, display and analysis. The following figures show screen shots of the instruments set-up window and results while running spectra. Digitizer control and data analysis is performed using a customized program that was developed using LabVIEW.